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Investigation of mechanism of antiwear additives by means of computer simulation

コンピュータシミュレーションを利用した耐摩耗添加剤のメカニズムの検討

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Abstract

Antiwear properties of phoshphonic acid derivatives in trimethylolpropane esters were investigated under boundary conditions. Effect of molecular structure of phoshphonic acid derivative on antiwear properties was observed. The computer assisted chemistry was applied to explain the phenomena. Dipole moment of individual additives was calculated by means of molecular orbital method. Good relationship of dipole moment of the derivatives with their antiwear properties was found. Antiwear properties of dialkyl phosphonates depend on polarity of base fluid. Nonpolarity index (NPI) of trimethylolpropane ester molecule was calculated to explain the phenomena. The trimethylolpropane esters have NPI in the range of 34.3 - 185.5. Dialkyl phosphonates provide good antiwear properties in less polar trimethylolpropane esters (higher NPI), whereas their antiwear properties are not sufficient in polar trimethylolpropane esters (lower NPI). Antiwear properties of dialkyl phosphonates in formulated trimethylolpropne esters were also investigated. Dialkyl phosphonates provide good antiwear properties in less polar formulated oils, whereas their antiwear properties are not sufficient in polar formulated oils. Therefor, amine salts of phosphonic acid were designed as new antiwear additive system for polar trimethylolpropane esters. Dipole moment of these salts was much higher than that of phosphonates. Excellent antiwear properties of the salts was confirmed even in polar base fluid.

Keywords : synthetic esters, antiwear additives, phosphonates, dipole moment, nonpolarity index, computer assisted chemistry, amine salts of phosphonic acid

注意：本稿中では, 本文中で説明していない専門用語は「(*数字)」で示し, 本稿末に説明文を掲載した.